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Summary

A general, analytical model for the dry friction of two atomically flat surfaces has been developed by combining existing models of dislocation drag with grain-boundary theory and co-incident site lattice theory. The model, which has no adjustable parameters, gives numbers for the dynamic friction which are within a factor of 2-3 of experimental results in ultra-high vacuum and is in qualitative agreement with a number of other experimental results such as frictional anisotropy, temperature dependence and the formation of transfer layers. Of particular importance, since the model is analytic, not numerical, it has predictive power including the effect of sliding velocity and temperature. It is hoped that this model will be a first step towards a general understanding of the role of dislocation drag in solid-solid friction and will stimulate further extensions, for instance to look at the role of barriers at the interface.

A few experiments have also been conducted to measure friction properties at and near special misfit angles (analogous to grain boundaries in bulk). Friction studies have been carried out on sodium chloride and strontium titanate.

Work started during the previous grant on quasicrystalline thin films has been completed.

Friction between atomically flat surfaces: Theory

Friction is a pervasive phenomenon, which is estimated to represent an economic cost of approximately $100 billion/year in the U.S. alone, and an estimated 1.6% of developed countries' GDP[1]. Although the importance of friction, and reducing it, was recognized as far back as the construction of the pyramids, we still have only a very fragmented basic understanding of the atomic mechanisms. Various models have been proposed[2, 3] of which the most widely used is the Frenkel-Kontorova approach[3]. In this model one of the two materials is represented by a periodic potential, and the other by a set of atoms connected by simple springs (or more complicated functional forms) to the other material. As the two bodies slide past each other the motion of the atoms in the potential leads to the forces associated with friction. More complicated and complete models, in principle somewhat similar, have been developed using atomistic approaches including molecular dynamics[4, 5]. These, however, are currently computationally limited to short time scales and small sizes.

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13. ABSTRACT *(Maximum 200 Words)*

An analytical model for dry friction using a combination of dislocation drag and solid-solid interface theory was developed. This model, with no adjustable parameters, gives semi-quantitatively correct numbers for experimental friction coefficients in ultra-high vacuum, and is also consistent with a number of other experimental finding ranging from the formation of contact layers to temperature dependence. Experiments on macroscopic single crystals to explore the angular dependence of solid-solid friction were performed, and found to be consistent with theoretical predictions albeit complicated by noise in the measurements.

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We have developed a different approach to the same problem. A brief report has been submitted [6], and a more detailed explanation is being prepared for publication. Our model uses an analytical approach, rather than a numerical one. In many respects the Frenkel-Kontorova model is the grandfather of contemporary models of dislocations in materials. If this model is used for two different materials, the problem is equivalent to the classic problem of misfit dislocations which was solved first by Frank and van der Merwe[7] using a variant of the Frenkel-Kontorova equations. If the two materials are in relative motion, the interface can be modeled in terms of the motion of misfit dislocations and dissipative forces expressed in terms of understood equations for dislocation drag[8-14]. We argue that to account for the relative misorientation of the two bodies one should apply modern grain and interface boundary theory, particularly the coincident site lattice approach[15-17]. Without any adjustable parameters we are able to obtain estimates, in an analytical form, for the friction between two materials in terms of some of the basic physical properties. While the model is too simple to represent a real material where many other effects such as third-bodies are critical[18, 19], we believe it serves as a useful general step in understanding friction.

The general form for a friction force derived from the dragging of dislocations between two flat contacting crystalline surfaces was solved to be

$$F_{macro} = \frac{\sigma_P A}{\gamma} coth\left(\frac{2b\sigma_P \gamma sin\frac{\Delta\theta}{2}}{BV}\right)$$

where σ_P is the Peierls stress, A is the dislocation array length, b the Burgers vector, V is the surface sliding velocity, and $\gamma=\sin(\theta)+\cos(\theta)$. Here, θ is the absolute in-plane misorientation angle and $\Delta\theta$ is the angular increment by which the orientation differs from specific coincident site orientations (Σ boundaries). The γ term arises from the orthogonal distribution of Burgers vectors in a lattice for a cubic twist interface. The dependence on the misorientation angle is shown in the following graph, for arbitrary units of force. The four lowest index coincident site boundaries are displayed in Figure 1.

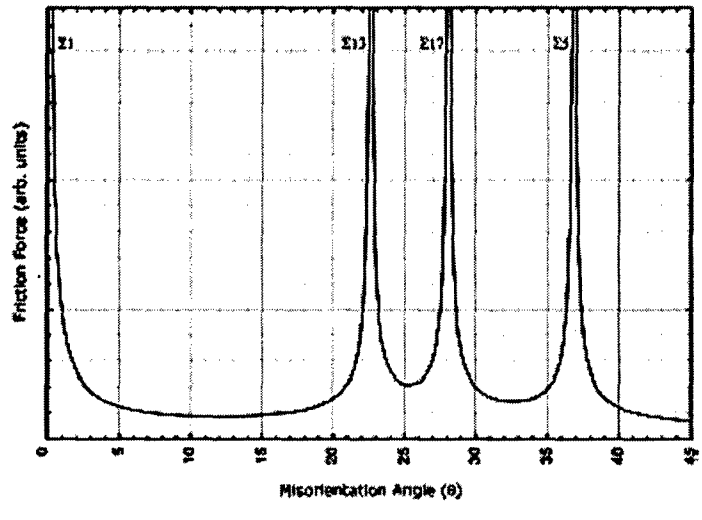

Figure 1: Theoretical Friction versus misorientation angle

Many more basic predictions lie within this general model. For instance, the dependence on sliding velocity is shown in Figure 2 below for different temperatures. A transition between nearly constant force with velocity to a region of viscous behavior is seen, and can be completely characterized by simple materials properties. The viscous domain, where force is linearly proportional to the sliding velocity, arises from phonon and electron drag contributions to the sliding interfacial dislocations. A convergence to the Peierls stress is a natural consequence of viscous drag terms giving way to a radiative term at low velocities [14].

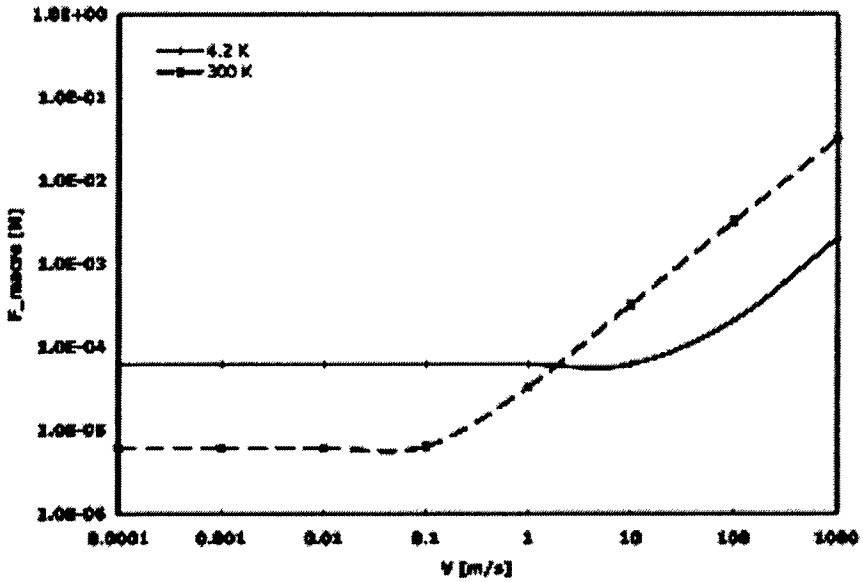

Figure 2: Calculated sliding force versus velocity at two different temperatures

The real power of this model lies in its analytical form. Using no adjustable parameters, we are able to estimate friction coefficients to within factors or two or three of comparable UHV friction studies. These estimates incorporate Hertzian-like contact models for multiasperity contact to predict the contact area where dislocation drag forces act as the single contributor to friction. Calculated friction coefficients for Cu and Ni yield 19.30 and 30.95, respectively. Full parameterization can be referenced in our submitted manuscript [6]. This model will form an initial step in characterizing friction on an atomic scale, not with absolute numerical accuracy, as friction encompasses many phenomena, but with physical trends that are useful in understanding friction at its most fundamental level.

Atomic Scale Friction: Experiments

Friction measurements have been carried out to identify lattice contributions to atomic-scale friction. Following the assumption that certain twist grain boundary configurations can be extended to increased interfacial sliding resistance, we have seen encouraging evidence that small angular misorientations may significantly contribute to elements of friction when regarding interfacial commensurability. Studies have first been carried out in the case of multi-asperity

contact in ambient conditions in a pin-on-disk configuration. To further increase angular resolution and to approach a more defined, crystalline-crystalline contact, nanoindentation instrumentation has been outfitted for these measurements.

NaCl single crystals were freshly cleaved, exposing a fresh (001) surface. This cleaved crystal was placed as the disk in a standard pin-on-disk arrangement. In place of a pin, a smaller polished (rounded, radius ~ 1cm) (001) surface of NaCl was used. Sliding tests at loads of 50 mN were performed several times for each angular increment of 0.3 degrees. Average friction coefficients were calculated and summarized for increasing and decreasing misorientation angle and are shown below.

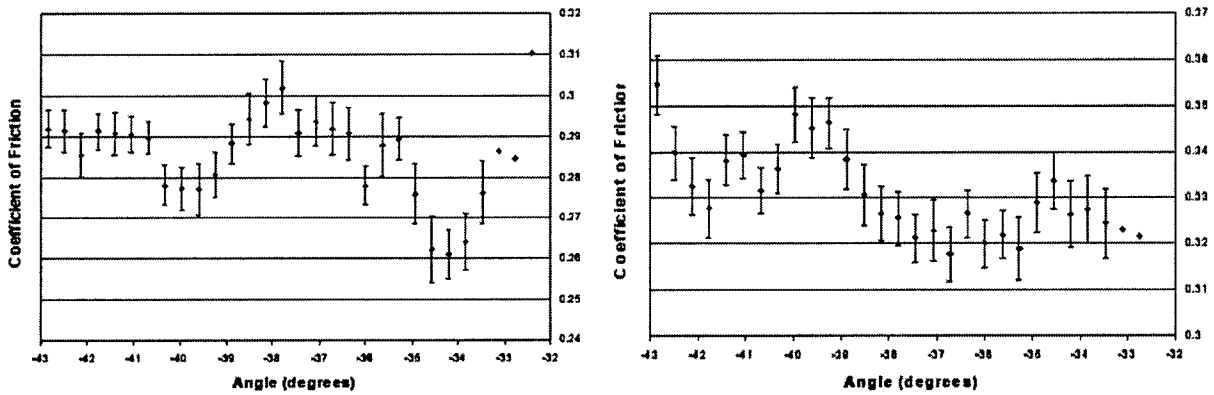

Figure 3: Experimental friction coefficient force versus angle, increasing (right) and decreasing (left)

The measured friction coefficient values correspond closely with the angular spacings and absolute orientations matching the Σ5 and Σ53 grain boundaries. Since a peak in friction is seen in each independent measurement, this leads us to believe that a coincident site lattice contribution is present in sliding friction as is relevant in interfacial grain boundary studies, where adhesion is strong. This prediction is developed more thoroughly in our analytical friction theory.

In order to repeat the experiment on a finer load and size scale and without the extreme sensitivity to humidity as shown by NaCl crystals, strontium titanate ($SrTiO_3$) single crystals (MTI Crystal, Inc.) were used. Friction experiments were carried out in collaboration with Hysitron, Inc. The UB1 nanomechanical test instrument system was used to measure the friction force between two finely epi-polished (100)-oriented $SrTiO_3$ crystals. The instrument uses a three-plate capacitive force sensing mechanism with a load noise floor of 100 nN. A tip was fabricated in a manner that preserved the original polish (<0.6 nm RMS roughness) of the (100) surface, but reduced the polished tip area to 2000 square microns. Scratch tests were carried out at a load of 800 micronewtons at angular intervals of 1 degree and a sliding speed of 10 microns per second. Relative humidity in the testing enclosure was monitored at a constant 18%.

Inspection of the samples via optical and atomic force microscopy of the crystalline surface following the tests showed no signs of wear. Friction data was collected through 100 degrees of misfit - keeping the sliding direction constant - and analyzed for trends. Structure to the data was observed (Figure 4), showing areas of increased friction at angular increments consistent with a majority of low index coincident site boundaries. This result is consistent with our analytical theory of dragging dislocations at sliding interfaces.

A more detailed look at Figure 4 shows that the predicted relative misorientation angle matches the spectrum of coincident boundaries where the corresponding friction peaks exist. The 45° local minimum is surrounded by equally spaced peaks that lie precisely on the Σ5 and Σ17 boundaries for cubic twist boundary systems. Similar behavior is seen in the vicinity of the Σ1 configuration. This data suggests that the dependence of friction on crystalline structure, and particularly the motion of dislocations, is present and is a significant contributor to the fundamental understanding of sliding interfaces.

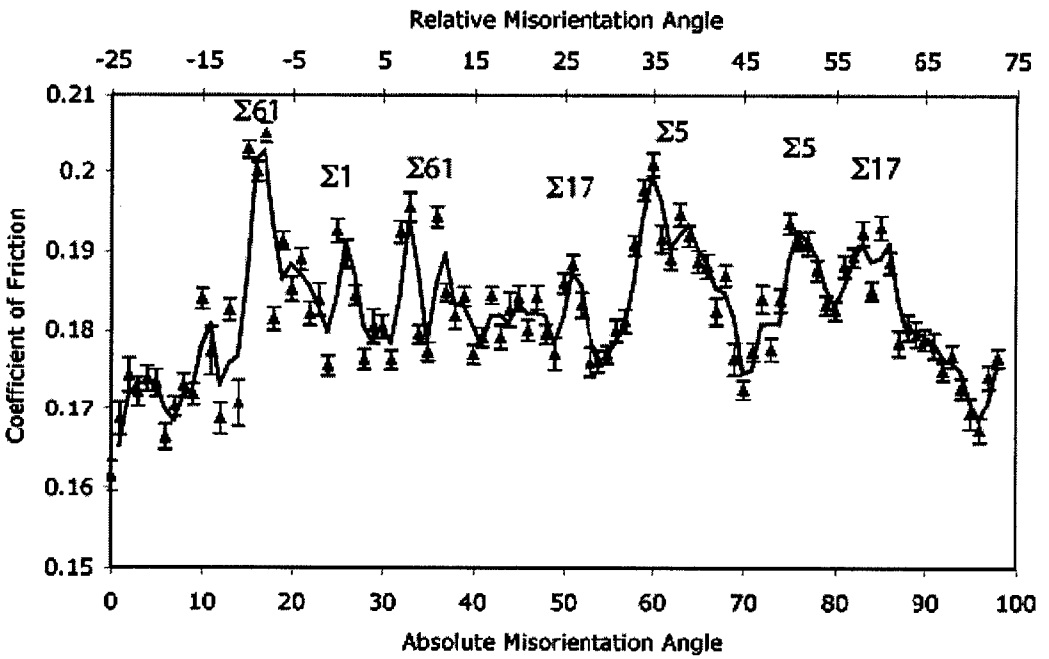

Figure 4: Experimental friction coefficient force versus angle for $SrTiO_3$

Further experiments to are scheduled in collaboration with Hysitron, Inc. These experiments will be run at a higher load in order to increase the anisotropic response. Care must be taken, however, not to enter the regime where plastic deformation dominates friction. An amorphous material will also be used as a reference for one half of the sliding interface, in order to isolate anisotropic contributions. As in all of these experiments, it is of great importance to control the environmental conditions (humidity) as well as surface roughness, contact alignment and sliding speed.

Growth of Quasicrystalline Thin Films

Some elements of work on quasicrystalline thin films were started under prior funding, and were completed within this grant. The main effort was generalizing out earlier model for epitaxy of quasicrystalline thin films on single crystal substrate to successfully explaining all published observations of crystalline-quasicrystalline interface configurations. This is significant in that verifying that crystalline-quasicrystalline interfaces obey rules similar to those for crystalline-crystalline interfaces connects to existing mathematical models of incommensurate interfaces where it has been speculated that below the Aubry transition there can be zero static friction.

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2. *A. Merkle and L. D. Marks, A Dislocation Drag Model for Friction, Physical Review Letters, Submitted (2005)*
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